

Density of States Modulations from Oxygen Phonons in d -wave Superconductors: Reconciling Angle-Resolved Photoemission Spectroscopy and Scanning Tunneling Microscopy

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Scanning tunneling microscopy (STM) measurements have observed modulations in the density of states (DOS) of a number of high- T_c cuprates. These modulations have been interpreted in terms of electron-boson coupling analogous to the dispersion “kinks” observed by angle-resolved photoemission spectroscopy (ARPES). However, a direct reconciliation of the energy scales and features observed by the two probes is presently lacking. In this paper we examine the general features of el-boson coupling in a d -wave superconductor using Eliashberg theory, focusing on the structure of the modulations and the role of self energy contributions λ_z and λ_ϕ . We identify the features in the DOS that correspond to the gap-shifted bosonic mode energies and discuss how the structure of the modulations provides information about an underlying pairing mechanism and the pairing nature of the boson. We argue that the scenario most consistent with the STM data is that of a low-energy boson mode renormalizing over a second dominant pairing interaction and we identify this low-energy mode as the out-of-phase bond buckling oxygen phonon. The influence of inelastic damping on the phonon-modulated DOS is also examined for the case of $\text{Bi}_2\text{Si}_2\text{CaCu}_2\text{O}_{8+\delta}$. Using this simplified framework we are able to account for the observed isotope shift and anti-correlation between the local gap and mode energies. Combined, this work provides a direct reconciliation of the bandstructure renormalizations observed by both ARPES and STM in terms of coupling to optical oxygen phonons.

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I. INTRODUCTION

In conventional superconductors, the role of electron-phonon (el-ph) interactions as the pairing “glue” was confirmed by the observation of fine-structure in the tunneling-derived density of states (DOS).^{1,2} In the cuprates, a great deal of effort has been expended in search of similar signatures using different probes.^{3–35} The observation of a particular mode, be it spin or lattice, might be used to infer the nature of the principal pairing mediator. However, to date, there is no consensus on the existence of such a mode³⁶ and if it does exist, whether it is tied to the lattice or spin degrees of freedom.

Electronic renormalizations in the form of dispersion “kinks” have also been observed in the electronic dispersion of the cuprates by angle-resolved photoemission spectroscopy (ARPES).^{6–8,11,13–18} Occurring at an energy scale $\sim 65 - 70$ meV in the nodal direction $(0,0) - (\pi,\pi)$ of the Brillouin zone, these kinks have been interpreted as coupling to a bosonic mode of either an electronic^{6–12} or lattice origin.^{13–21} According to Eliashberg theory, the position of a kink due to coupling to a sharp bosonic mode in a d -wave superconductor is expected to occur at an energy of $\Delta_0 + \Omega_0$, where Ω_0 is the energy of the mode and Δ_0 is the maximum value of the d -wave gap.^{2,16,34} With this observation, the energy of the mode responsible for the kink has been estimated at $\sim 35 - 40$ meV. This energy coincides with the energies

of the spin-resonance mode centered at $\mathbf{Q} = (\pi/a, \pi/a)$ observed by neutron scattering³⁷ and the out-of-plane “ B_{1g} ” bond buckling oxygen modes.¹⁵ As a result, there is considerable debate as to the identity of the underlying mode, however the observation of multiple mode coupling in some cuprates,^{20,21,28} as well as recent measurements of an isotope effect for the kink energy,¹⁴ provide strong evidence for the phonon interpretation of the ARPES renormalizations. However, regardless of the identity of the boson, the $\sim 35 - 40$ meV energy scale extracted from ARPES data appears to be in conflict with the ~ 52 meV energy scale extracted from STM by Lee *et al.*³ Therefore it is an open question as to whether the two experimental probes are observing different mode couplings or if they are reflecting different manifestations of the same bosonic mode.

Microscopic inhomogeneities in the local density of states (LDOS) which is proportional to the derivative of the tunneling current $N(\omega) \propto dI/dV$, as well as signatures of coupling to a bosonic mode, have been observed in scanning tunneling microscopy (STM) experiments on $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (Bi-2212).^{3–5} In Ref. 3, estimates for the local gap size are determined from the peak-to-peak distance of the coherence peaks while the energy of the bosonic mode is identified as the energy position of a peak in d^2I/dV^2 measured relative to the energy of the superconducting gap. While the positions of the superconducting coherence peaks vary at different tip locations, estimates for the mode energy are inversely correlated

with the local gap size and the distribution of mode estimates, centered at ~ 52 meV, shows a clear isotope shift upon ^{18}O substitution. The energy of the bosonic mode also appears to be immune to doping while the spectra changes qualitatively. These observations are inconsistent with a coupling to the spin resonance mode,³⁵ and points to a lattice origin for the mode involving oxygen vibrations.

Fine structures in the DOS of a number of additional cuprates have been reported by other STM and SIS junction tunneling measurements, each producing different estimates for mode energies. A structure similar to that reported for Bi-2212 has been reported in $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10+\delta}$ (Bi-2223),²² with the energy scale of the mode estimated at ~ 35 meV. It is important to note that in Ref. 22 the mode energy was associated with the position of the minima in the LDOS (root in d^2I/dV^2) relative to the local gap size as opposed to Ref. 3, which extracted the mode estimate from the peak in dI/dV^2 . Bicrystal grain boundary SIS junction measurements on optimal doped $\text{La}_{1.84}\text{Sr}_{0.16}\text{CuO}_4$ thin films observe modulations in the DOS which correspond well with peaks in the neutron derived phonon spectra,²³ and in agreement with the multiple features present in ARPES data.²⁸ Examinations of tunneling data on $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO) and the electron doped system $\text{Pr}_{0.88}\text{LaCe}_{0.12}\text{CuO}_4$ have produced a similar correspondence between modulations in the DOS and phonon density of states in these materials.^{24,25} The observation of multiple mode coupling, as well as the fact that the spin resonance is well separated in energy from the phonons in the electron doped systems provide further evidence that the spin resonance mode is unlikely to be the source of these features as proposed by Ref. 35. However, the question remains whether coupling to the mode can be cast in the usual form for el-ph coupling to oxygen modes, as inferred from ARPES^{15,19}, or whether the structure in the LDOS could be due to phonon-assisted co-tunneling from the tip via the apical atom.²⁷

Co-tunneling via a strong local coupling of electrons in the STM tip to the apical atom imparts structure in the form of peaks in the dI/dV at an energy scale of $\Delta_0 + \Omega$ and multiples of the phonon frequency $\Delta_0 + 2\Omega$, $\Delta_0 + 3\Omega$, ... even though the coupling of the planar superconducting electrons to the apical atom may be weak.^{27,38} However, recent observations of charge-ordering structures via Fourier transform spectroscopy in Bi-2212,³⁹ which has apical oxygen atoms, and $\text{Ca}_{2-x}\text{Na}_x\text{CaO}_2\text{Cl}_2$,⁴⁰ which doesn't, empirically indicate that no one particular matrix element controls the tunneling pathway along the c -axis. If a single pathway were to dominate the tunneling process one would expect the charge ordering features in these two materials to have qualitatively different structures.

In light of these observations we investigate the role of el-ph coupling between planar oxygen vibrations and the electrons of the CuO_2 plane. The aim of this paper is twofold. First, due to the discrepancies in the struc-

tures in dI/dV used to extract boson mode energies in previous works, we examine the qualitative signatures of el-boson coupling in a d -wave superconductor. In doing so, we explicitly determine which features in dI/dV (or d^2I/dV^2) are best identified with the energy of the boson mode. Furthermore, we demonstrate how the qualitative structure in dI/dV can be used to determine if the mode coupling is the predominant pairing mechanism. We argue that most consistent interpretation of the STM data is that of a low-energy mode renormalizing over a dominant high-energy (or instantaneous) pairing interaction. In this case, the mode energy should be extracted from a *minimum* in $N(\omega) \propto dI/dV$. In light of this finding, the mode energy estimate from Ref. 3 is revised to $\sim 35 - 45$ meV, in agreement with Ref. 22 and the energy scale extracted from ARPES measurements.^{16,21} The second goal of this paper is to demonstrate that the modulations in $N(\omega)$ can be understood in terms of the same el-ph coupling models that have been successful in accounting for the dispersion “kinks” observed ubiquitously in the cuprates by ARPES. Combined, these calculations demonstrate a unified picture of el-ph coupling in the cuprates probed by both STM and ARPES.

The organization of this paper is as follows. In section II the Eliashberg framework for calculating the self-energy due to el-boson coupling in a d -wave superconductor is reviewed. In section III focus is placed on el-boson contributions in multiple momentum channels in order to demonstrate the qualitative changes in the self-energy that are expected for a mode which couples differently in each of the momentum channels. We find that these considerations are critical and can qualitatively change the structure of the boson modulations in the DOS, altering the feature in dI/dV corresponding to the mode energy. This aspect of the calculation has generally been neglected in previous Eliashberg treatments,^{12,29-31} where the boson contribution to the single-particle (λ_z) and anomalous (λ_ϕ) self-energies have been taken to be equal to (or proportional to) one another over the entire energy range of the boson spectrum. For an s -wave superconductor $\lambda_z = \lambda_\phi$ but for a d -wave superconductor $\lambda_z \neq \lambda_\phi$ and usually $\lambda_z \gg \lambda_\phi$ in modes derived from the strong Coulomb repulsion having strong onsite (λ_z) and near-neighbor (λ_ϕ) interactions. Next, having established the role of the symmetry channels, we then turn to the qualitative differences in the el-boson structures in the infinite and finite band formalisms of Eliashberg theory. Since the cuprates have a relatively narrow bandwidth due to the Cu $3d$ character of the $pd\text{-}\sigma^*$ band, one expects that the latter case is the more appropriate formalism for these materials. Finally, in section IV we present a model calculation for the el-ph modulated LDOS in Bi-2212. Here it is demonstrated that the DOS modulations can be reproduced using coupling strengths similar to those used in previous ARPES treatments.¹⁵ We then introduce a phenomenological treatment of local damping effects reflecting the inhomogeneity observed in Bi-2212 and the associated broadened spectral features.⁴

This model is able to reproduce the anticorrelation between the local superconducting gap estimates and local mode estimates. Finally, the reported isotope shift of the distribution mode estimates is naturally captured by the el-ph coupling model, as our calculation explicitly show. We then end with a brief summary and discussion about the implications of this work.

II. ELECTRON-BOSON COUPLING

In Migdal-Eliashberg theory, which neglects crossing diagrams, the self-energy due to el-boson coupling is given by

$$\hat{\Sigma}(\mathbf{k}, i\omega_n) = \frac{1}{N\beta} \sum_{\mathbf{q}, m} \int_0^\infty d\nu \frac{2\nu\alpha^2 F(\mathbf{k}, \mathbf{q}, \nu)}{\nu^2 + (\omega_m - \omega_n)^2} \times \hat{\tau}_3 \hat{G}(\mathbf{p}, i\omega_m) \hat{\tau}_3 \quad (1)$$

where ω_m (ω_n) is a Boson (Fermion) Matsubara frequency, and $\alpha^2 F(\mathbf{k}, \mathbf{q}, \nu) = -|g(\mathbf{k}, \mathbf{q})|^2 \text{Im} D(\mathbf{q}, \nu)$ is the effective electron-boson spectral function. Here, the vertex $g(\mathbf{k}, \mathbf{q})$ gives the strength of scattering of the electron from state \mathbf{k} to $\mathbf{p} = \mathbf{k} - \mathbf{q}$ and $D(\mathbf{q}, i\omega_m)$ is the boson propagator.

In the superconducting state, the electron propagator $\hat{G}(\mathbf{k}, i\omega_n)$ is given by

$$\hat{G}^{-1}(\mathbf{k}, i\omega_n) = i\omega_n Z(\mathbf{k}, i\omega_n) \hat{\tau}_0 + [\epsilon_{\mathbf{k}} + \chi(\mathbf{k}, i\omega_n)] \hat{\tau}_3 + \phi(\mathbf{k}, i\omega_n) \hat{\tau}_1. \quad (2)$$

Here, the self-energy has been divided into the canonical form²

$$\hat{\Sigma}(\mathbf{k}, i\omega_n) = i\omega_n [1 - Z(\mathbf{k}, i\omega_n)] \hat{\tau}_0 + \chi(\mathbf{k}, i\omega_n) \hat{\tau}_3 + \phi(\mathbf{k}, i\omega_n) \hat{\tau}_1 \quad (3)$$

where $i\omega_n [1 - Z(\mathbf{k}, i\omega_n)]$ and $\chi(\mathbf{k}, i\omega_n)$ are the odd and even components of the electron self-energy, respectively, and $\phi(\mathbf{k}, i\omega_n)$ is the anomalous self-energy. Eqs. (1) - (3) can now be self-consistently solved on the Matsubara frequency axis. An analytic expression for the self-energy on the real axis can be derived from these equations by explicitly performing the analytic continuation $i\omega_n \rightarrow \omega + i\delta$, where $\delta > 0$ is an infinitesimal real number. The single-particle DOS is $N(\omega)$ is obtained from the electron Green's function $N(\omega) = -2 \sum_{\mathbf{k}} \text{Im} G_{11}(\mathbf{k}, \omega) / \pi$.

Marsiglio *et al.*⁴¹ have developed an efficient iterative procedure for performing the analytic continuation of the el-boson self-energy. In this formalism $\hat{\Sigma}(\mathbf{k}, \omega)$ is obtained by iteratively solving^{41,42} ($\mathbf{p} = \mathbf{k} - \mathbf{q}$)

$$\begin{aligned} \hat{\Sigma}(\mathbf{k}, \omega) = & \frac{1}{N\beta} \sum_{\mathbf{q}} \sum_{m=0}^{\infty} \lambda_0(\mathbf{k}, \mathbf{q}, \omega - i\omega_m) \hat{\tau}_3 \hat{G}(\mathbf{p}, i\omega_m) \hat{\tau}_3 \\ & + \frac{1}{N} \sum_{\mathbf{q}} \int_{-\infty}^{\infty} d\nu \alpha^2 F(\mathbf{k}, \mathbf{q}, \nu) \times \\ & [n_b(\nu) + n_f(\nu - \omega)] \hat{\tau}_3 \hat{G}(\mathbf{p}, \omega - \nu) \hat{\tau}_3 \end{aligned} \quad (4)$$

where n_b and n_f are the Bose and Fermi factors, respectively, and

$$\lambda_0(\mathbf{k}, \mathbf{q}, \omega) = \int_0^\infty d\nu \alpha^2 F(\mathbf{k}, \mathbf{q}, \nu) \frac{2\nu}{\omega^2 - \nu^2}.$$

In evaluating Eq. (4), the solution to the imaginary axis equations $\hat{\Sigma}(\mathbf{k}, i\omega_n)$ are used as input and $\hat{\Sigma}(\mathbf{k}, \omega)$ is solved for iteratively.⁴¹

In large bandwidth systems the momentum sum is typically evaluated by assuming a linear band near the Fermi level $\epsilon_{\mathbf{k}} = (k - k_F) \cdot v_F$ (with v_F the Fermi velocity), replacing the normal state density of states $N(\omega)$ with its value at the Fermi level $N(0)$ and extending the limits of the energy integral to infinity.⁴¹ (Note that in this approximation $\chi(\mathbf{k}, \omega)$ is featureless and only contributes to an overall shift of the chemical potential.²) For brevity we refer to this approximation as the “infinite band” formalism of Eliashberg theory.

III. QUALITATIVE SIGNATURES OF EL-BOSON COUPLING

Before turning to the model calculations, let us discuss the qualitative signatures of el-boson coupling in a d -wave superconductor. We would like to examine coupling in various momentum channels and, to this end, the coupling constant can be expanded in terms of Brillouin zone harmonics

$$|g(\mathbf{k}, \mathbf{q})|^2 = \sum_{J, J'} Y_J(\mathbf{k}) |g_{J, J'}|^2 Y_{J'}(\mathbf{k} - \mathbf{q}) \quad (5)$$

where the sum J runs over the irreducible representations of the point group of the crystal. We assume $g_{J, J'}$ is diagonal in this basis and identify $J = 0$ and $J = 2$ with the s and $d_{x^2-y^2}$ symmetries. If one then only admits the gap solution in the $J = 2$ channel, the energy and momentum dependence of the self-energies are factorable with $Z(\mathbf{k}, \omega) = Z(\omega) Y_0(\mathbf{k})$, $\chi(\mathbf{k}, \omega) = \chi(\omega) Y_0(\mathbf{k})$ and $\phi(\mathbf{k}, \omega) = \phi(\omega) Y_J(\mathbf{k})$, where $J = 0, 2$ for each symmetry.

The overall strength of the el-boson coupling in momentum channel J can be parameterized by the dimensionless constant λ_J

$$\lambda_J = \int_0^\infty \frac{2d\nu}{\nu} \frac{\sum_{\mathbf{k}, \mathbf{q}} \alpha^2 F(\mathbf{k}, \mathbf{q}, \nu) Y_J(\mathbf{k}) Y_J(\mathbf{p}) \delta(\epsilon_{\mathbf{k}}) \delta(\epsilon_{\mathbf{p}})}{\sum_{\mathbf{k}} Y_J(\mathbf{k})^2 \delta(\epsilon_{\mathbf{k}})}. \quad (6)$$

It is important to note that $\lambda_{J=0} \equiv \lambda_z$ ($Y_0(\mathbf{k}) = 1$) characterizes the contribution to the el-boson self-energies $Z(\mathbf{k}, \omega)$ and $\chi(\mathbf{k}, \omega)$ while $\lambda_{J=2} \equiv \lambda_\phi$ ($Y_2 = [\cos(k_x a) - \cos(k_y a)]/2$) characterizes the contribution to $\phi(\mathbf{k}, \omega)$ for a $d_{x^2-y^2}$ superconductor. The relative values of $\lambda_{z, \phi}$ also determine the transition temperature T_c , which, in the

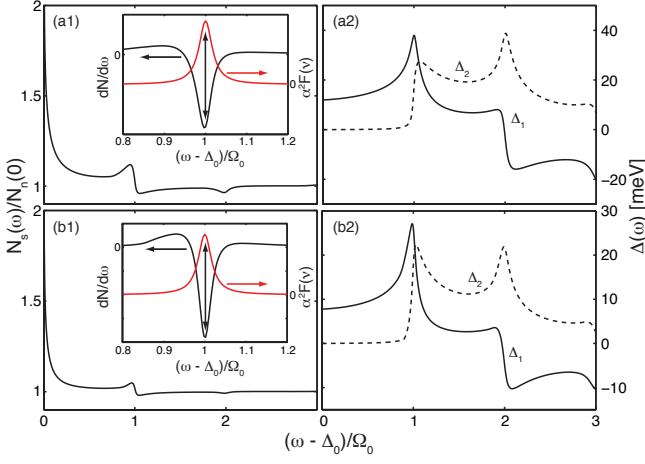


FIG. 1: (Color online) (a1), (a2) The DOS $N(\omega)$ and corresponding real and imaginary parts of the gap function $\Delta(\omega)$, respectively, for an s -wave superconductor coupled to a single bosonic mode. (b1), (b2) $N(\omega)$ and $\Delta(\omega)$ for a d -wave superconductor with $\lambda_z = 1.6$ and $\lambda_\phi = 0.8\lambda_z$. The insets of panels (a1),(b1), show $dN/d\omega$ and $\alpha^2 F(\nu + \Delta_0)$ in order to highlight the correspondence between features in the DOS and peaks in the boson spectrum. The secondary structure in $\Delta(\omega)$ at $\omega = \Delta_0 + 2\Omega_0$ are due to self-energy effects due to two-phonon processes.

limit of weak coupling is given by

$$k_b T_c = 1.13 \hbar \Omega_0 \exp \left[-\frac{1 + \lambda_z}{\lambda_\phi} \right]. \quad (7)$$

The relative magnitudes of $\lambda_{z,\phi}$ can also affect the qualitative signatures of the boson modulations in the density of states.

In the superconducting state, neglecting the role band-structure, the DOS $N_s(\omega)$ can be written as

$$\frac{N_s(\omega)}{N_n(0)} = \text{Re} \left\langle \frac{\omega}{\sqrt{\omega^2 - \Delta^2(\mathbf{k}, \omega)}} \right\rangle \quad (8)$$

where $N_n(0)$ is the density of states at the Fermi level and $\Delta(\mathbf{k}, \omega) = \phi(\mathbf{k}, \omega)/Z(\mathbf{k}, \omega) = \Delta_1(\mathbf{k}, \omega) + i\Delta_2(\mathbf{k}, \omega)$ is the complex momentum-dependent gap function and $\langle \dots \rangle$ denotes an average over the Fermi surface.² In what follows, the notation Δ_0 is introduced for the maximum value of the superconducting gap on the Fermi surface, which is defined by the value of the gap function at the gap edge $\Delta_0 = \Delta(\mathbf{k}_f^{\text{AN}}, \omega = \Delta_0)$, where \mathbf{k}_f^{AN} is the Fermi momentum along the zone face $(0,0)-(\pi,0)$.

For $\omega \gg \Delta_0$, Eq. (8) can be expanded yielding²

$$\frac{N_s(\omega)}{N_n(0)} = 1 + \frac{1}{2\omega^2} \langle \Delta_1^2(\mathbf{k}, \omega) - \Delta_2^2(\mathbf{k}, \omega) \rangle. \quad (9)$$

From Eq. (9) it is clear that the phononic substructure is given by the frequency dependence of the $\Delta(\mathbf{k}, \omega)$, which is obtained by evaluating Eq. 4. In Figs. 1a1-a2 we plot

$N_s(\omega)$ and the corresponding $\Delta(\omega)$, respectively, for an isotropic s -wave superconductor. Here, we have assumed a single bosonic mode with a Lorentzian spectral density, characterized by a half-width at half-maximum of $\Gamma_b = 1$ meV and centered at $\Omega_0 = 52$ meV (inset of panel Fig. 1a1). The overall coupling strength has been set to $\lambda_z = 0.8$.

As $\omega \rightarrow \Delta_0 + \Omega_0$, the real part of $\Delta(\omega)$ begins to rise producing an enhancement in the DOS for $\omega \lesssim \Delta_0 + \Omega_0$. At $\Delta_0 + \Omega_0$ the real part begins to drop while the imaginary part experiences a sudden rise due to Kramers-Kronig consistency. This results in a rapid suppression in the DOS at this energy scale, which drives the DOS below its bare value. As a result, the energy scale $\Delta_0 + \Omega_0$ manifests as a shoulder in $N(\omega)$ or a minimum in $dN/d\omega$, as shown in the inset of Fig. 1a1. This is the classic McMillan-Rowell signature, similar to that observed in Pb, where phonons are solely responsible for pairing.^{1,2} In the case of a d -wave superconductor the situation is nearly identical when $\lambda_z = \lambda_\phi = 0.8$, and the magnitude of the gap function is comparable to that obtained for the s -wave case with a similar value of λ_z (not shown). Again, since the contribution from the boson is equal in the two channels, the boson energy scale manifests as a shoulder on the low-energy side of the modulation. This signature qualitatively unchanged when $\lambda_z > \lambda_\phi$, as shown in Figs. 1b1,b2 for $\lambda_z = 1.6$, $\lambda_\phi = 0.8\lambda_z$, with the overall magnitude of $\Delta(\omega)$ reduced by a factor of 2. The reduction in $\Delta(\omega)$ illustrates the importance of the relative magnitudes of λ_z and λ_ϕ .

We now consider the case of a low-energy boson which renormalizes over a second mode, higher in energy and dominant in its contribution to pairing. We associate this high energy mode with spin fluctuations with a broad Lorentzian spectral density centered at $\Omega_{sf} \sim 2J = 260$ meV and with $\Gamma_{sf} = 30$ meV. The total coupling to this mode is taken to be $\lambda_{sf,z} = \lambda_{sf,\phi} = 1.6$. For the low-energy boson we take $\Gamma_b = 0.5$ meV, $\lambda_z = 1.6$ and $\lambda_\phi = 0$.

The results for the two-mode calculation are shown in Fig. 2. The structure of the renormalizations in this case differs considerably and the shoulder on the low energy side of the renormalization is significantly less pronounced. Here, the sharper spectral density and increased value of λ_z for the low-energy mode are required in order to accentuate the weak low-energy feature. Without this increased coupling the low-energy renormalizations are difficult to resolve. In the Eliashberg formalism, a high energy boson produces a gap function whose real part is relatively frequency independent for energies on the order of lower energy mode Ω_b , while an instantaneous pairing interaction produces a frequency independent gap function up to an energy scale set by the Coulomb interaction.⁴³ Therefore, assuming a frequency independent pair field ϕ_0 , modulated by el-boson coupling, we write

$$\frac{\phi(\omega)}{Z(\omega)} = \frac{\phi_0 + \delta\phi(\omega)}{Z_0 + \delta Z(\omega)} = \frac{\phi_0}{Z_0} \frac{1 + \delta\phi/\phi_0}{1 + \delta Z/Z_0}$$

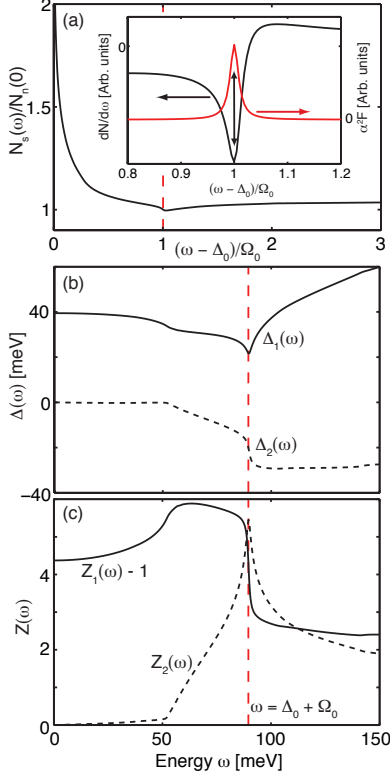


FIG. 2: (Color online) (a) $N(\omega)$ for a d -wave superconductor where the $\Omega \sim 52$ meV mode ($\lambda_{b,z} = 1.6$, $\lambda_{b,\phi} = 0$) renormalizes over a dominate mode associated with spin fluctuations with $\Omega_{sf} = 260$ meV ($\lambda_{sf,z} = \lambda_{sf,\phi} = 1.6$). Inset: $dN/d\omega$ and $\alpha^2 F(\nu - \Delta_0)$ highlighting the correspondence between the low-energy mode and structure in $N(\omega)$. (b), (c) $\Delta(\omega)$ and $Z(\omega)$ for this case. The red dashed lines indicate the energy of $\Delta_0 + \Omega_0$ where Ω_0 is the energy of the center of the low-energy spectra density (inset, panel (a)).

where $\delta\phi$ and δZ are the el-boson contributions to the self-energy. The DOS (for $\omega \gg \Delta_0$) can then be written as

$$\frac{N_s(\omega)}{N_f} = 1 + \frac{\Delta_0^2}{2\omega^2} \left(1 - \frac{\delta\phi(\omega)}{\phi_0} - \frac{\delta Z(\omega)}{Z_0} \right). \quad (10)$$

If the el-boson contribution to pairing is small, as is the case in Fig. 2, $\delta\phi$ can be neglected and one sees that the fine structure tracks the structure of $\delta Z(\omega)$ (Fig. 2c). In Fig. 2b, this is seen as the suppression of $\Delta_1(\omega)$ as $\omega \rightarrow \Delta_0 + \Omega_0$ and results in a dip structure in $N(\omega)$ (Fig. 2a) with no pronounced shoulder on the low-energy side of the renormalization. We also note that the boson energy scale remains as the minima in $dN/d\omega$ (inset of Fig. 2a).

Experimentally, the modulations in the tunneling spectra appear as a dip-hump structure with no pronounced shoulder on the low-energy side of the modulations.^{3,22} We therefore conclude that, within validity of Eliashberg theory, the bosonic mode responsible for the LDOS renormalizations cannot be the sole contributor to pairing in

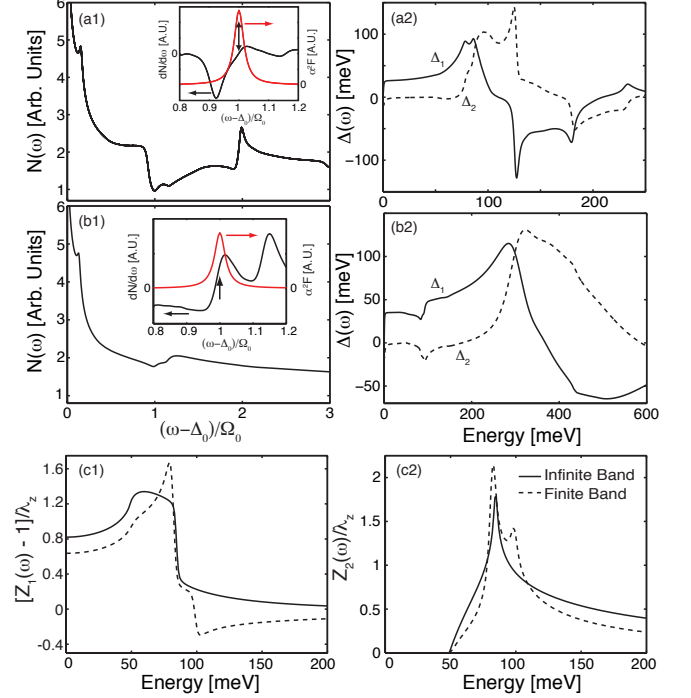


FIG. 3: (Color online) The structures in the DOS $N(\omega)$ and gap function $\Delta(\omega)$ when the structure of the bare band has been retained. (a1),(a2) $N(\omega)$ and $\Delta(\omega)$, respectively, for a d -wave superconductor coupled to a single low-energy mode which provides all of the pairing. (b1),(b2) $N(\omega)$ and $\Delta(\omega)$ for the two mode case analogous to the case shown in Figs. 1c1,c2. The insets of panels (a1) and (b1) show $dN/d\omega$ and the low energy component of $\alpha^2 F(\nu + \Delta_0)$ in order to show the correspondence between structure in $N(\omega)$ and peaks in $\alpha^2 F(\nu)$. (c1), (c2) The real and imaginary parts of $Z(\omega)$ calculated in the infinite- (solid) and finite-band (dashed) Eliashberg formalisms. Here, a single iteration of the Eliashberg equations has been assumed with coupling to an Einstein mode centered at $\Omega = 52$ meV and assuming a d -wave gap with $\Delta_0 = 35$ meV.

the cuprates otherwise a pronounced shoulder on the low-energy side of the renormalization would be present. More likely, the low-energy boson renormalizes over the dominant source of pairing. This approach has been invoked previously in order to account for the ARPES kinks since the value of $\lambda_z \sim 0.3 - 0.5$ needed to reproduce the kink is too small to provide enough pairing to account for the large gap values.^{19,34}

Although the two mode picture can account for the lack of shoulder feature in the LDOS in the infinite band formalism, the hump structure on the high-energy side of the renormalizations is absent. This is due to the approximations inherent to the formalism used so far, which neglect the role of both bandstructure and the narrow bandwidth of the system. In Fig. 3 solutions to the Eliashberg equations given by Eq. (4), which retain the full \mathbf{k} -dependence of the band structure, are shown. Again, two cases are considered in analogy to Figs. 1 and

2: a single mode with $\lambda_z = 1.9 = \lambda_\phi$, $\Gamma = 1$ meV, and $\Omega_0 = 52$ meV, and a two-mode case with the modes parameterized by $\Omega_{b,sf} = 52, 300$ meV $\Gamma_{b,sf} = 1, 30$ meV, $\lambda_{z,sf} = \lambda_{\phi,sf} = 1.7$, $\lambda_{z,b} = 0.52$ and $\lambda_{\phi,b} = 0$. In order to model a realistic bandstructure for the low energy dispersion have assumed a 5-parameter tight-binding model obtained from fits to the low-energy dispersion observed by ARPES.⁴⁴ Fig. 3a1, a2, show $N(\omega)$ and $\Delta(\omega)$, respectively, for the single low-energy mode which is pairing, analogous to Fig. 1, while Fig. 3b1,b2 shows the results for the two mode calculation, analogous to Fig. 2.

The first observation is that the shoulder feature remains when a single mode contributes significantly to pairing, while a pronounced dip-hump structure is produced when the mode renormalizes over another dominant mechanism. In the latter case the hump is more pronounced due to the additional self-energy contributions when scattering to the large DOS near the van Hove. In the cuprates the energy of the phonons (and spin resonance mode) lie close in energy to both the superconducting gap Δ_0 and the van Hove energy $\epsilon(0, \pi/a)$. Because of this near degeneracy of energy scales there is an overall enhancement of the self-energy due to the increased density of states to which the bosons can couple anti-nodal region. This degeneracy has also been noted in studies on the temperature dependence of the el-ph self-energy observed by ARPES.^{15,16} To illustrate this point, in Fig. 3c1,c2 compares the real and imaginary parts of $Z(\omega)$ in the two formalisms. (In order to compare comparable cases $Z(\omega)$ as been calculated assuming a single iteration of the Eliashberg equations and the results have been normalized by the value of λ_z .) When the bandstructure has been retained $Z(\omega)$ (as well as χ and ϕ) develops additional structure and $Z_1(\omega)$ becomes negative at energies larger than $E(0, \pi) + \Omega_0$, where $E^2(0, \pi) = \epsilon^2(0, \pi) + \Delta^2(0, \pi)$ is the energy of the quasiparticle at the van Hove singularity, resulting in the hump structure observed in $N(\omega)$. If the bandstructure is neglected $Z_1(\omega)$ remains positive and smoothly approaches zero as $\omega \rightarrow \infty$. One can therefore conclude that the structure in the underlying band can contribute to the structure in the self-energy and must be considered in realistic treatments of narrow bandwidth systems such as the cuprates.

The second observation made of Fig. 3 is that the correspondence between the minima in $dN/d\omega$ and peaks in $\alpha^2 F$ no longer holds for a d -wave superconductor with a finite bandwidth (insets of Figs. 3a1 and b1). For the single-mode model the peak in $\alpha^2 F(\nu)$ corresponds to the minimum in $N(\omega)$ or the root in $dN/d\omega$ while for the two-mode model this energy scale does not correspond to *any* feature in $dN/d\omega$. For the choice of $\alpha^2 F$ and $\epsilon_{\mathbf{k}}$ used here, the energy scale $\Delta_0 + \Omega_0$ is located between the root and maximum in $dN/d\omega$ and either energy scale gives a reasonable estimate for the mode energy.

We also note the presence of secondary features in the DOS at an energy $E(0, \pi) + \Omega_0$ which is absent when momentum structure of the band is neglected. The pres-

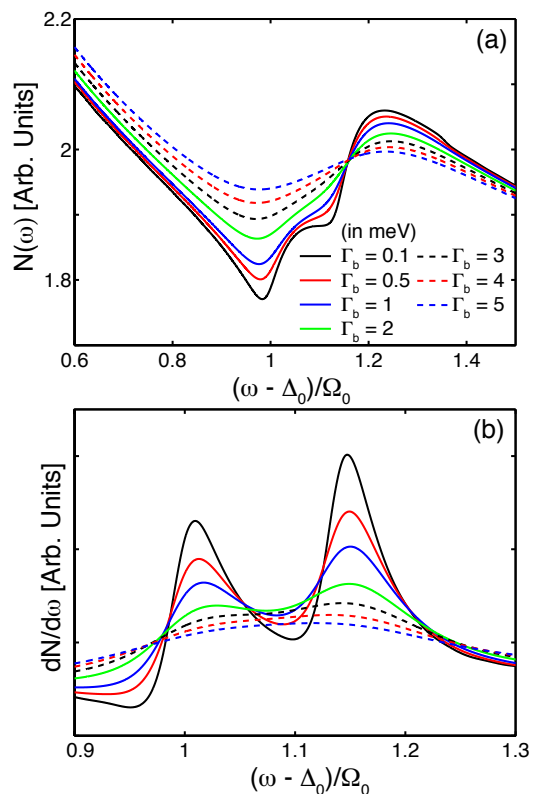


FIG. 4: (Color online) (a) $N(\omega)$ and (b) $dN/d\omega$ for ω in the neighbourhood of the low-energy boson renormalizations for various values of the low-energy mode's spectral width Γ_b (in meV).

ence of this feature can complicate the identification of the mode energy if the boson spectral density is broad enough. In Fig. 4 $N(\omega)$ and $dN/d\omega$ are plotted for the two-mode model for various values of the low-energy mode's spectral width Γ_b . Here, we have kept the details of the high-energy mode fixed to the same values used in Fig. 3 and adjusted the strength of λ_b such that the total value of $\lambda_{z,\phi}$ are fixed. As the value of Γ_b is increased, the width of the structure in $N(\omega)$ is increased and eventually becomes broad enough that the double dip structure merges into a single dip-hump feature. As a result, the peaks in $dN/d\omega$ merge into a single peak whose maximum occurs between $\Omega_0 + \Delta_0$ and $\Omega_0 + E(0, \pi)$. The maximum in $dN/d\omega$ is very sensitive to the width of the boson spectrum as well as the energy of the van Hove and is therefore an unreliable indicator of the boson mode energy. However, the position of the root in $dN/d\omega$ on the low energy side of the renormalizations is much less sensitive to these factors. Although this feature slightly underestimates the mode energy, it does appear to be a robust indicator of the mode energy.

The qualitative change in the phonon fine-structure is the central result of this paper. It reconciles the discrepancy in the ~ 52 meV scale observed in STM³ and the ~ 70 meV “kink” observed by photoemission in Bi-

2212.¹⁵ In Ref. 3 the maxima in $d^2I/dV^2 \propto dN/d\omega$ was taken for the mode estimate, corresponding to the shoulder of the dip-hump structure of the DOS. However, as shown above, the energy scale of the mode is more accurately given by the minimum (the dip) in $N(\omega)$ (or a root in d^2I/dV^2), this choice results in an overestimate of the mode energy. A closer examination of Fig. 1 of Ref. 3 reveals that the minima in the DOS is ~ 15 -20 meV lower in energy. This brings the mode estimate in line with the energy of the B_{1g} modes invoked to explain the kink in the nodal region of superconducting Bi-2212. Indeed, Ref. 22 has tracked the minimum in the related Bi-2223 system, which also has strong coupling to the B_{1g} modes, and obtained a mode energy of 35 meV, consistent with our findings. The qualitative difference in structure also provides a pathway to experimentally distinguish between fine structure due to co-tunneling effects, where a maximum in $N(\Omega_0 + \Delta_0) \propto dI/dV|_{\omega=\Omega_0+\Delta_0}$ occurs, and intrinsic el-boson coupling where a minimum is expected if the mode is not dominating pairing, or a shoulder is expected if the mode is contributing heavily to pairing.

IV. CONSIDERATIONS FOR BI-2212

We now turn to a model calculation for Bi-2212. Here we consider coupling to the out-of-phase Cu-O bond buckling B_{1g} phonon branch, previously invoked to explain the renormalization in the bandstructure of Bi-2212 observed by ARPES.¹⁵ Since we are now concerned with how the phonons renormalize over a dominant interaction we consider only a single iteration of the Eliashberg equations and treat the phonon mode as a dispersionless Einstein mode with $\Omega_0 = 36$ meV. This treatment is identical to that used in previous works examining the dispersion kinks observed by ARPES.^{15,16,19} For simplicity, we expand the coupling constant as $|g(\mathbf{k}, \mathbf{q})|^2 = g_z^2 + g_\phi^2 Y_d(\mathbf{k})Y_d(\mathbf{p})$ and set $g_{z,\phi}$ such that $\lambda_{z,\phi} = 0.31, 0.1$, comparable to the values obtained in previous works.¹⁵ After analytic continuation, the zero-temperature expressions for the imaginary parts of the self-energies are:

$$\begin{aligned} \omega Z_2(\mathbf{k}, \omega) &= \frac{\pi}{2N} \sum_{\mathbf{p}} |g(\mathbf{k}, \mathbf{q})|^2 \delta(E_{\mathbf{p}} + \Omega_0 - \omega) \quad (11) \\ \chi_2(\mathbf{k}, \omega) &= -\frac{\pi}{2N} \sum_{\mathbf{p}} |g(\mathbf{k}, \mathbf{q})|^2 \frac{\epsilon_{\mathbf{p}}}{E_{\mathbf{p}}} \delta(E_{\mathbf{p}} + \Omega_0 - \omega) \\ \phi_2(\mathbf{k}, \omega) &= \frac{\pi}{2N} \sum_{\mathbf{p}} |g(\mathbf{k}, \mathbf{q})|^2 \frac{\Delta_{\mathbf{p}}}{E_{\mathbf{p}}} \delta(E_{\mathbf{p}} + \Omega_0 - \omega) \end{aligned}$$

which are evaluated for $\omega > 0$. Here, $E(\mathbf{k}) = \sqrt{\epsilon^2(\mathbf{k}) + \Delta^2(\mathbf{k})}$. The real-part of the self-energies are obtained via the Kramers-Kronig relations. In these calculations the superconducting gap Δ_0 is taken as an input parameter and we supplement the real part of ϕ in order to maintain the value of the gap at the gap edge.^{19,34} Finally, an intrinsic damping $\Gamma = 5$ meV, independent of ω and \mathbf{k} , is added to the imaginary part of $Z(\mathbf{k}, \omega)$.

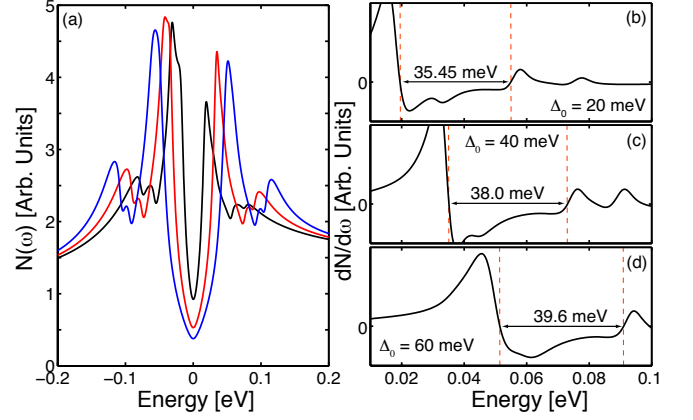


FIG. 5: (Color online) (a) The density of states calculated for coupling to the B_{1g} phonon branch at $T = 0$. Each spectra is calculated using a 5-parameter tight-binding bandstructure and a d -wave gap with $\Delta_0 = 20$ (black), 40 (red) and 60 (blue) meV. (b)-(d) $dN/d\omega$ for the indicated gap size. The red dashed lines indicate the position of the roots corresponding to estimates for Δ_0 and $\Delta_0 + \Omega_0$, respectively.

The DOS results are presented in Fig. 5, where we have chosen three different values of Δ_0 to mimic the variation in the LDOS observed in different regions of an optimally doped sample. The calculated DOS for the three gap values all show a clear dip in the spectra around $\Delta_0 + \Omega_0$ as well as the secondary structure at $E(0, \pi) + \Omega_0$ due to the van Hove singularity. We also note that the features associated with the phonon renormalizations are more pronounced due to the use of a sharp Einstein mode. Estimates are obtained empirically for the mode energy and gap size from the calculated DOS via the gap referencing procedure used in Ref. 4. In order to avoid complications associated with the van Hove singularity in determining the gap magnitude on the occupied side ($\omega < 0$) of the spectra we work on the hole side ($\omega > 0$) and identify the energy $\Delta_0 + \Omega_0$ with the root in $dN/d\omega$. When the gap referencing procedure is applied to the data, the resulting gap estimate is equal to the quadrature addition of the gap on the Fermi surface Δ_0 and the damping term Γ . The empirically determined mode energy is therefore underestimated since the effective mode position is $\Omega_0 + \Delta_0 - \sqrt{\Delta_0^2 + \Gamma^2}$. Since we have used a constant value of Γ for each value of Δ_0 , the small gap data has a larger ratio of Γ/Δ_0 , and thus the extracted mode energy systematically deviated from Ω_0 .

A constant value of Γ does not capture the local inhomogeneity of the parameters entering into the DOS itself. Specifically, we now modify the magnitude of the el-ph coupling and inelastic damping Γ included in both the spectral function and evaluation of the self-energy, as a function of gap size. We naïvely associate the larger gap with “underdoped” regions which, due to the reduction in screening of the el-ph interaction, leads to an increase in the relative strength of the coupling with gap

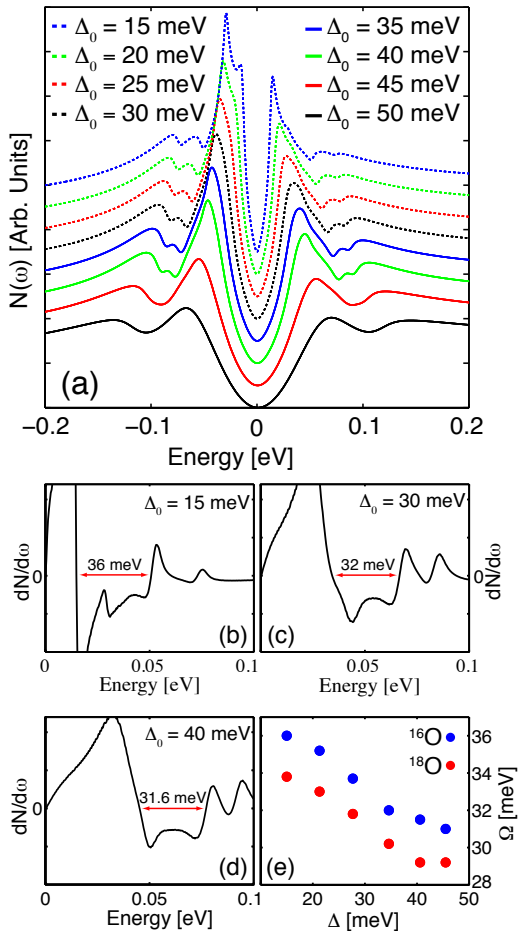


FIG. 6: (Color online) A waterfall plot of $N(\omega)$ calculated for doping values spanning the large gap to small gap regions. Each DOS was calculated for coupling the same mode used in Fig. 5. The gap values indicated in the legend denote the input values of Δ_0 . (b),(c),(d) $dN/d\omega$ for selected DOS presented in panel (a) for the hole side ($\omega > 0$) of the spectrum. The red arrows indicate the roots used to estimate the energies Δ_0 and $\Delta_0 + \Omega_0$. (e) The mode energy estimate obtained from the position of the local minima relative to the coherence peak. The blue data points correspond to data for ^{16}O simulations while the red data points correspond to ^{18}O simulations.

size. At the same time, damping effects are taken to increase together with the gap size to mimic the crossover to smeared gap structures found in the large gap regions. This is modeled as an increasing ratio of Γ/Δ_0 in the large gap region. The DOS was then recalculated for input gap values ranging from 15 to 50 meV.

The new DOS spectra obtained are presented in Fig. 6a. For small gap inputs one can see sharp coherence peaks followed by a well defined dip-hump structure associated with the el-ph coupling. For larger gaps, the associated larger damping smears the coherence peaks and they are washed away for $\Delta_0 = 50$ meV. The gap and phonon energy scales can now be extracted from $dN/d\omega$,

which are shown for selected spectra in Figs. 6b-d. The resulting correlation between the extracted Δ_0 and Ω_0 are shown Fig. 6e (blue dots). The anti-correlation which emerges between the two energies stems from the progressive underestimation of the mode energy as the gap size and Γ are increased.

In order to model the isotope effect, these calculations were repeated with adjustments appropriate for the replacement of ^{16}O with ^{18}O . Specifically, this includes a shift in the phonon frequency by a factor of $\sqrt{M_{16}/M_{18}}$ and a decrease in the overall coupling by a factor $(M_{16}/M_{18})^{1/4}$. (This substitution leaves the values of $\lambda_{z,\phi}$ unchanged.) The red data points of Fig. 6e show the correlation between the estimate for Ω and Δ_0 obtained for ^{18}O upon repetition of the previous calculations. In both cases, the anti-correlation persists and a clear isotope shift can be seen, which is on the order of that observed and that one would expect based on the known shift in the phonon energy. The overall agreement with the experimental data is good, and the anti-correlation can be accounted for relatively well by incorporating damping effects into a simple el-ph picture.

V. CONCLUSIONS

We have examined the signatures of el-boson coupling in a d -wave superconductor when the boson mode does not provide the dominate pairing interaction. The resulting fine structure for the modulations in the DOS are qualitatively different than those found in the conventional s -wave superconductors. We found that the manifestation of bosonic energy scales in the LDOS depends on an interplay between the strength of the el-boson coupling in each momentum channel, as well as the details of the underlying bandstructure. In order to reproduce the spectra observed experimentally by STM we found that both the full structure of the band, as well as the differing contributions of λ_z and λ_ϕ for the boson mode in question have to be accounted for. Taking these considerations into account, the 52 meV scale reported in Ref. 3 is found to be an overestimate of the mode energy and instead, the local minima in $N(\omega)$ should be considered. The mode energy extracted from the minima of the spectra reported in Ref. 3 agrees well with the energy of the B_{1g} phonon modes as well as a more recent measurements reported for Bi-2223.²² This fact reconciles the scales observed by STM with those observed in numerous ARPES experiments. With the revised estimate for the mode energy, we then calculated the LDOS including coupling to the B_{1g} phonon modes. Using a simple consideration for the local intrinsic damping we found that the model is able to reproduce both the structure of the renormalizations and the observed anti-correlation between the extracted values of Ω_0 and Δ_0 . The success of the el-ph model in accounting for the data obtained by both probes provides further evidence in support of the phonon interpretation of the electronic renormalizations

observed now in both ARPES and STM experiments.

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